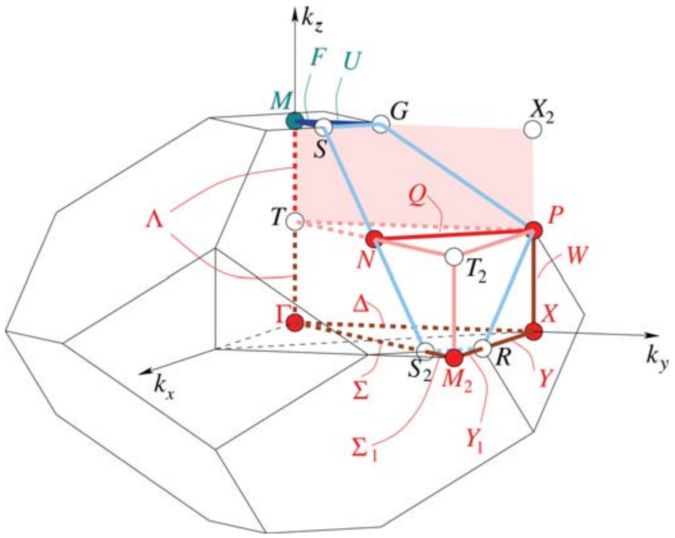

Fig. 1.5.5.4. Brillouin zone with asymmetric unit and representation domain of CDML for arithmetic crystal class $4/mmmI$: $c/a > 1$. Space groups $I4/mmm - D_{4h}^{17}$ (139) to $I4_1/acd - D_{4h}^{20}$ (142). Reciprocal-space group $(I4/mmm)^*$, No. 139: $c^*/a^* < 1$ (see Table 1.5.5.4). The representation domain of CDML is different from the asymmetric unit. Auxiliary points: X_2: $0, \frac{1}{2}, \frac{1}{2}$; T: $0, 0, \frac{1}{4}$; T_2: $\frac{1}{2}, \frac{1}{2}, \frac{1}{4}$. Flagpole: $[T\,M]$ $0, 0, z$: $\frac{1}{4} < z < \frac{1}{2}$. Wing: $[T\,P\,X_2\,M]$ $0, y, z$: $0 < y < \frac{1}{2}, \frac{1}{4} < z < \frac{1}{2}$.

Example. In Table 1.5.5.3 one finds for the arithmetic crystal class $4/mmmI$ of space groups:

$$B \quad \alpha, \beta, -\alpha \quad 16\ m\ ..m \quad x, x, z\text{: } [\Gamma\, M\, Z_2\, Z_0]$$

The parameter description would be:

$$x, x, z\text{: } 0 < x < \tfrac{1}{2},\ 0 < z \le z_0 - 2x(2z_0 - \tfrac{1}{2})$$

Horizontal lines. The horizontal lines extending across the tables separate blocks with different numbers of free parameters. Decisive for this subdivision is the number of free parameters of the Wyckoff position to which the Wintgen position is assigned, not the number of free parameters of CDML.

Example. Arithmetic crystal class mm2F, see Table 1.5.5.5

The **k**-vector labels 'Γ $0, 0, 0$' and 'Z $\frac{1}{2}, \frac{1}{2}, 0$' of CDML have no free parameter. However, they correspond to the Wyckoff position '2 a $mm2$ $0, 0, z$', which has one free parameter. Therefore, Γ and Z are listed together with 'Λ $\alpha, \alpha, 0$' and 'LE $-\alpha, -\alpha, 0$' in the block for the symmetry lines, *i.e.* for the **k** vectors with one free parameter: in $(Imm2)^*$ there is no parameter-free Wintgen position at all.

The **k**-vector labels 'Σ $0, \alpha, \alpha$' and 'A $\frac{1}{2}, \frac{1}{2} + \alpha, \alpha$' of CDML have one free parameter each. However, they correspond together with other **k**-vector labels to the Wyckoff position '4 c $.m.$ $x, 0, z$'. Therefore, Σ and A are listed together with 'J $\alpha, \alpha + \beta, \beta$' and '$JA$ $-\alpha, -\alpha + \beta, \beta$' and others in the block for the planes, *i.e.* for the **k** vectors with two free parameters.

Table 1.5.5.4. *List of **k**-vector types for arithmetic crystal class $4/mmmI$: $c/a > 1$*

See Fig. 1.5.5.4. Wyckoff positions e and f exchanged. Parameter relations: $x = -\frac{1}{2}\alpha + \frac{1}{2}\beta$, $y = \frac{1}{2}\alpha + \frac{1}{2}\beta + \gamma$, $z = \frac{1}{2}\alpha + \frac{1}{2}\beta$.

k-vector label, CDML	Wyckoff position of *IT* A, *cf.* Section 1.5.4.3	Parameters
Γ $0, 0, 0$	2 a $4/mmm$	$0, 0, 0$
M $\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$	2 b $4/mmm$	$0, 0, \frac{1}{2}$
$M \sim M_2$		$\frac{1}{2}, \frac{1}{2}, 0$
X $0, 0, \frac{1}{2}$	4 c $mmm.$	$0, \frac{1}{2}, 0$
P $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	4 d $\bar{4}m2$	$0, \frac{1}{2}, \frac{1}{4}$
N $0, \frac{1}{2}, 0$	8 f $..2/m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
Λ $\alpha, \alpha, -\alpha$	4 e $4mm$	$0, 0, z$: $0 < z < \frac{1}{2}$
W $\alpha, \alpha, \frac{1}{2} - \alpha$	8 g $2mm.$	$0, \frac{1}{2}, z$: $0 < z < \frac{1}{4}$
Σ $-\alpha, \alpha, \alpha$	*ex* 8 h $m.2m$	$x, x, 0$: $0 < x \le s_2$
F $\frac{1}{2} - \alpha, \frac{1}{2} + \alpha, -\frac{1}{2} + \alpha$	*ex* 8 h $m.2m$	$x, x, \frac{1}{2}$: $0 < x < s = \frac{1}{2} - s_2$
$F \sim \Sigma_1 = [S_2\, M_2]$		$x, x, 0$: $s_2 < x < \frac{1}{2}$
$\Sigma \cup \Sigma_1 = [\Gamma M_2]$	8 h $m.2m$	$x, x, 0$: $0 < x < \frac{1}{2}$
Δ $0, 0, \alpha$	8 i $m2m.$	$0, y, 0$: $0 < y < \frac{1}{2}$
Y $-\alpha, \alpha, \frac{1}{2}$	*ex* 8 j $m2m.$	$x, \frac{1}{2}, 0$: $0 < x \le r$
U $\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} + \alpha$	*ex* 8 j $m2m.$	$0, y, \frac{1}{2}$: $0 < y < g = \frac{1}{2} - r$
$U \sim Y_1 = [R\, M_2]$		$x, \frac{1}{2}, 0$: $r < x < \frac{1}{2}$
$Y \cup Y_1 = [X\, M_2]$	8 j $m2m.$	$x, \frac{1}{2}, 0$: $0 < x < \frac{1}{2}$
Q $\frac{1}{4} - \alpha, \frac{1}{4} + \alpha, \frac{1}{4} - \alpha$	16 k $..2$	$x, \frac{1}{2} - x, \frac{1}{4}$: $0 < x < \frac{1}{4}$
C $-\alpha, \alpha, \beta$	*ex* 16 l $m..$	$x, y, 0$: $[\Gamma\, S_2\, R\, X]$
D $\frac{1}{2} - \alpha, \frac{1}{2} + \alpha, -\frac{1}{2} + \beta$	*ex* 16 l $m..$	$x, y, \frac{1}{2}$: $[M\, S\, G]$
$D \sim C_1$		$x, y, 0$: $[M_2\, R\, S_2]$
$C \cup C_1 = [\Gamma\, M_2\, X]$	16 l $m..$	$x, y, 0$: $0 < x < y < \frac{1}{2}$
B $\alpha, \beta, -\alpha$	16 m $..m$	x, x, z: $[\Gamma\, S_2\, S\, M]$
$B = B_1 \cup B_2$ $= [\Gamma\, S_2\, N\, T] \cup [T\, N\, S\, M]$		
$B_2 \sim B_3$		x, x, z: $[T_2\, N\, S_2\, M_2]$
$B_1 \cup B_3 = [\Gamma\, M_2\, T_2\, T]$	16 m $..m$	x, x, z: $0 < x < \frac{1}{2}, 0 < z < \frac{1}{4}$ $\cup$ $\cup$ $x, x, \frac{1}{4}$: $0 < x < \frac{1}{4}$
A α, α, β	*ex* 16 n $.m.$	$0, y, z$: $[\Gamma\, X\, P\, G\, M]$
E $\alpha - \beta, \alpha + \beta, \frac{1}{2} - \alpha$	*ex* 16 n $.m.$	$x, \frac{1}{2}, z$: $[X\, P\, R]$
$E \sim A_1$		$0, y, z$: $[X_2\, G\, P]$
$A \cup A_1 = [\Gamma\, X\, X_2\, M]$	16 n $.m.$	$0, y, z$: $0 < y, z < \frac{1}{2}$
GP α, β, γ	32 o 1	x, y, z: $0 < x < y < \frac{1}{2}$; $0 < z < \frac{1}{4}$ $\cup$ $\cup$ $x, y, \frac{1}{4}$: $0 < x < y < \frac{1}{2} - x$